

Full wwPDB X-ray Structure Validation Report (i)

Jul 10, 2024 – 01:09 am BST

PDB ID : 9FIL

Title: Crystal Structure of reduced NuoEF variant E222K(NuoF) from Aquifex ae-

olicus bound to NAD+

Authors: Wohlwend, D.; Friedrich, T.; Goeppert-Asadollahpour, S.

Deposited on : 2024-05-29

Resolution : 2.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.37.1

buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

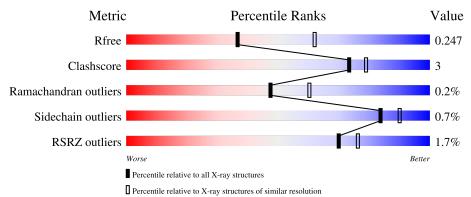
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	A	160	88%	9%	•
1	С	160	86%	11%	
2	В	434	88%	8%	
2	D	434	86%	10%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CL	D	505	-	-	X	-



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9682 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called NADH-quinone oxidoreductase subunit E.

\mathbf{Mol}	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace				
1	Δ	156	Total	С	N	О	S	0	0	0	
1	11	100	1268	821	204	234	9		O		
1	C	156	Total	С	N	O	S	0	0	0	
1	C	150	1268	821	204	234	9	0	U		

• Molecule 2 is a protein called NADH-quinone oxidoreductase subunit F.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	В	418	Total 3274	C 2103	N 548	O 609	S 14	0	2	0
2	D	418	Total 3268	C 2098	N 548	O 608	S 14	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	222	LYS	GLU	engineered mutation	UNP O66841
В	427	ALA	-	expression tag	UNP O66841
В	428	GLY	-	expression tag	UNP O66841
В	429	HIS	-	expression tag	UNP O66841
В	430	HIS	-	expression tag	UNP O66841
В	431	HIS	-	expression tag	UNP O66841
В	432	HIS	-	expression tag	UNP O66841
В	433	HIS	_	expression tag	UNP O66841
В	434	HIS	-	expression tag	UNP O66841
D	222	LYS	GLU	engineered mutation	UNP O66841
D	427	ALA	_	expression tag	UNP O66841
D	428	GLY	-	expression tag	UNP O66841
D	429	HIS	-	expression tag	UNP O66841
D	430	HIS	-	expression tag	UNP O66841
D	431	HIS	-	expression tag	UNP O66841
D	432	HIS	_	expression tag	UNP O66841

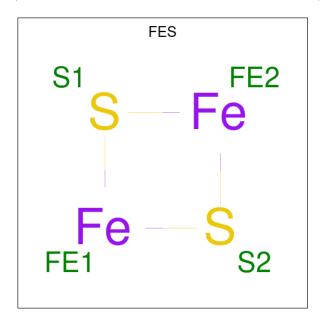
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Chain	Residue	Modelled	Actual	Comment	Reference	
D	433	HIS	-	expression tag	UNP O66841	
D	434	HIS	-	expression tag	UNP O66841	

 \bullet Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



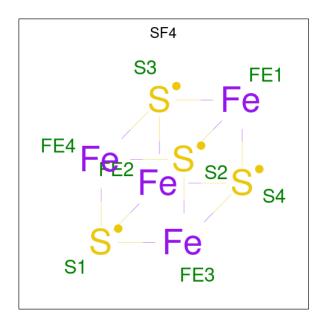
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	С	1	Total Fe S 4 2 2	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	В	5	Total Na 5 5	0	0
4	С	2	Total Na 2 2	0	0
4	D	2	Total Na 2 2	0	0

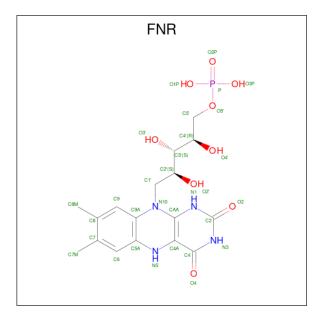
 \bullet Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Fe S 8 4 4	0	0
5	D	1	Total Fe S 8 4 4	0	0

• Molecule 6 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]P TERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR) (formula: $C_{17}H_{23}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms				ZeroOcc	AltConf
6	D	1	Total	С	N	О	Р	0	0
0	Б	1	31	17	4	9	1	U	0

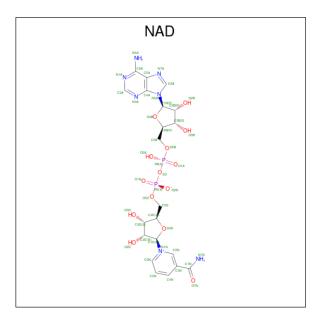
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Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
6	D	1	Total	С	N	О	Р	0	0
O	D	1	31	17	4	9	1	U	

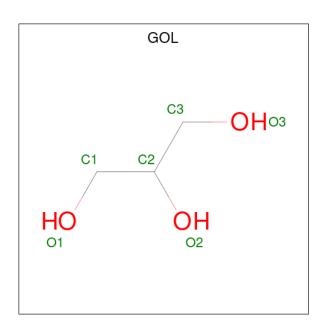
• Molecule 7 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	В	1	Total	С	N	О	Р	0	0
'	(D	1	36	15	6	13	2	U	
7	D	1	Total	С	N	О	Р	0	0
	1	33	14	5	12	2	U	0	

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total C O 6 3 3	0	0
8	В	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0

 \bullet Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Cl 1 1	0	0
9	D	2	Total Cl 2 2	0	0

• Molecule 10 is water.

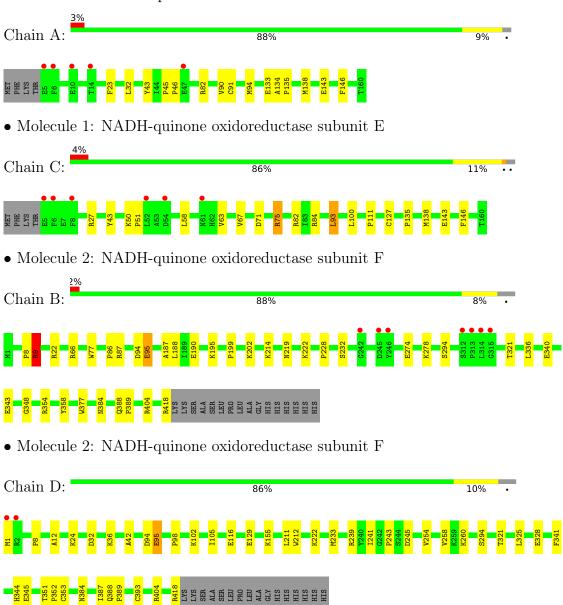
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	56	Total O 56 56	0	0
10	В	156	Total O 156 156	0	0
10	С	69	Total O 69 69	0	0
10	D	137	Total O 137 137	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADH-quinone oxidoreductase subunit E





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	64.14Å 115.54Å 189.92Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 - 2.54	Depositor
Resolution (A)	49.35 - 2.54	EDS
% Data completeness	99.0 (49.40-2.54)	Depositor
(in resolution range)	99.1 (49.35-2.54)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.32 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
D D.	0.201 , 0.248	Depositor
R, R_{free}	0.206 , 0.247	DCC
R_{free} test set	2370 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 32.6	EDS
L-test for twinning ²	$ < L >=0.52, < L^2>=0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9682	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 47.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6714e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FNR, NA, NAD, SF4, FES, CL, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.37	0/1297	0.71	0/1752	
1	С	0.39	0/1297	0.73	0/1752	
2	В	0.39	0/3353	0.74	0/4540	
2	D	0.40	0/3347	0.73	$1/4530 \ (0.0\%)$	
All	All	0.39	0/9294	0.73	1/12574~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	С	0	2
2	В	0	3
2	D	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	D	129	GLU	CB-CA-C	5.14	120.68	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	В	22	ARG	Sidechain
2	В	87	ARG	Sidechain
2	В	9	ARG	Sidechain
1	С	75	ARG	Sidechain
1	С	82	ARG	Sidechain
2	D	239	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1268	0	1269	8	0
1	С	1268	0	1269	11	0
2	В	3274	0	3227	22	0
2	D	3268	0	3227	25	0
3	A	4	0	0	0	0
3	С	4	0	0	0	0
4	A	1	0	0	0	0
4	В	5	0	0	0	0
4	С	2	0	0	0	0
4	D	2	0	0	0	0
5	В	8	0	0	0	0
5	D	8	0	0	0	0
6	В	31	0	22	0	0
6	D	31	0	22	0	0
7	В	36	0	20	0	0
7	D	33	0	16	0	0
8	В	12	0	16	2	0
8	D	6	0	8	0	0
9	В	1	0	0	0	0
9	D	2	0	0	2	0
10	A	56	0	0	0	0
10	В	156	0	0	1	0
10	С	69	0	0	1	0
10	D	137	0	0	1	0
All	All	9682	0	9096	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 3.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	$overlap(\AA)$
2:D:222:LYS:HE2	9:D:505:CL:CL	2.16	0.82
2:D:384:ASN:HD22	2:D:404:ARG:HH21	1.35	0.73
2:D:222:LYS:CE	9:D:505:CL:CL	2.78	0.68
2:B:202:LYS:HD3	10:B:645:HOH:O	1.98	0.62
2:D:233:MET:HE1	2:D:241:ILE:HD11	1.81	0.62
2:B:384:ASN:HD22	2:B:404:ARG:HH21	1.49	0.60
1:C:93:LEU:HD21	2:D:325:LEU:HG	1.86	0.56
2:B:377:TRP:CZ2	2:B:418:ARG:HG2	2.42	0.54
2:B:343:GLU:HG3	2:B:358:TYR:HA	1.92	0.52
1:C:75:ARG:HD2	10:C:344:HOH:O	2.09	0.51
1:A:43:TYR:O	1:A:45:PRO:HD3	2.10	0.51
2:B:77:TRP:HE1	2:B:219:ASN:ND2	2.10	0.50
2:B:336:LEU:O	2:B:340:GLU:HG3	2.12	0.50
2:B:9:ARG:HD2	2:D:155:LYS:O	2.13	0.49
2:B:77:TRP:HE1	2:B:219:ASN:HD21	1.58	0.49
2:D:353:CYS:HA	2:D:387:ILE:HG23	1.96	0.48
1:A:90:VAL:O	1:A:94:MET:HG2	2.15	0.47
2:B:190:GLU:OE1	2:B:195:LYS:HE2	2.14	0.47
1:A:138:MET:HG2	1:A:143:GLU:HG3	1.96	0.46
2:B:348:GLY:HA2	2:B:354[B]:ARG:HB2	1.97	0.46
2:D:294:SER:HA	2:D:321:THR:O	2.15	0.46
2:D:102:LYS:HD2	2:D:222:LYS:HE3	1.98	0.46
1:C:127:CYS:SG	2:D:98:PRO:HA	2.56	0.45
1:C:100:LEU:HD22	1:C:111:PRO:HG3	1.98	0.45
1:A:91:CYS:HA	1:A:134:ALA:HB1	1.98	0.45
2:D:94:ASP:O	2:D:95:GLU:C	2.54	0.45
2:B:294:SER:HA	2:B:321:THR:O	2.16	0.45
2:D:341:PHE:O	2:D:345:GLU:HG2	2.17	0.45
2:B:187:ALA:HB2	2:B:199:PRO:HG3	1.98	0.45
2:B:94:ASP:O	2:B:95:GLU:C	2.55	0.45
2:D:388:GLN:N	2:D:389:PRO:CD	2.80	0.45
1:C:71:ASP:OD2	2:D:344[B]:HIS:CE1	2.71	0.44
2:B:228:PRO:HB3	8:B:504:GOL:H32	1.99	0.44
2:D:243:PRO:HB2	2:D:245:ASP:OD1	2.18	0.44
1:C:135:PRO:HG2	1:C:146:PHE:HB3	2.00	0.44
2:D:254:VAL:HG12	2:D:258:VAL:HG21	1.99	0.43
2:D:42:ALA:HB3	2:D:116:GLU:OE2	2.19	0.43
1:C:84:ARG:HB2	1:C:138:MET:HB2	2.00	0.43

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A + 1	A4 0	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:A:23:PHE:HE2	1:A:32:LEU:HD12	1.83	0.43
1:C:143:GLU:HB3	2:D:8:PRO:HD3	2.01	0.43
2:D:102:LYS:O	2:D:105:ILE:HG12	2.18	0.43
1:C:50:LYS:N	1:C:51:PRO:HD2	2.34	0.42
2:B:86:PRO:HD2	2:B:214:LYS:HE2	2.02	0.42
2:B:274:GLU:O	2:B:278:LYS:HB3	2.19	0.42
2:D:328:GLU:HB2	10:D:658:HOH:O	2.20	0.42
1:A:135:PRO:HG2	1:A:146:PHE:HB3	2.02	0.41
2:D:211:LEU:HG	2:D:212:TRP:CD1	2.56	0.41
2:B:188:LEU:C	2:B:188:LEU:HD23	2.41	0.41
1:C:63:VAL:O	1:C:67:VAL:HG23	2.20	0.41
2:D:260:LYS:HB3	2:D:260:LYS:HE2	1.92	0.41
2:D:32:ASP:O	2:D:36:LYS:HG3	2.20	0.41
2:B:377:TRP:CH2	2:B:418:ARG:HG2	2.55	0.41
2:D:12:ALA:HB3	2:D:24:LYS:HA	2.02	0.41
1:A:133:GLU:HG3	2:B:8:PRO:HB2	2.02	0.41
1:C:27:ARG:HB2	1:C:58:LEU:HD11	2.02	0.41
2:D:351:THR:HB	2:D:352:PRO:HD3	2.02	0.41
2:B:66:ARG:HB3	2:B:222:LYS:HE2	2.02	0.40
1:A:45:PRO:HA	1:A:46:PRO:HD3	1.96	0.40
2:B:388:GLN:N	2:B:389:PRO:CD	2.85	0.40
2:B:228:PRO:CB	8:B:504:GOL:H32	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	154/160 (96%)	150 (97%)	4 (3%)	0	100	100
1	С	154/160 (96%)	148 (96%)	6 (4%)	0	100	100
2	В	418/434 (96%)	405 (97%)	12 (3%)	1 (0%)	47	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	417/434 (96%)	406 (97%)	10 (2%)	1 (0%)	47 60
All	All	1143/1188 (96%)	1109 (97%)	32 (3%)	2 (0%)	47 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	95	GLU
2	D	95	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	A	142/146~(97%)	142 (100%)	0	100	100
1	\mathbf{C}	$142/146 \ (97\%)$	140 (99%)	2 (1%)	67	79
2	В	336/357~(94%)	334 (99%)	2 (1%)	86	92
2	D	337/357 (94%)	334 (99%)	3 (1%)	78	86
All	All	957/1006~(95%)	950 (99%)	7 (1%)	84	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	9	ARG
2	В	232	SER
1	С	43	TYR
1	С	93	LEU
2	D	1	MET
2	D	393	CYS
2	D	418	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	39	ASN
2	В	198	HIS
2	В	220	ASN
2	В	384	ASN
1	С	17	GLN
1	С	62	HIS
2	D	220	ASN
2	D	286	ASN
2	D	384	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Ch		Res	Link	Bo	ond leng	ths	В	ond ang	les
IVIOI	туре	Chain	nes	2 LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FNR	D	502	-	32,33,33	0.43	0	40,50,50	0.55	0
5	SF4	D	501	2	0,12,12	-	-	-		
7	NAD	D	503	-	30,35,48	0.70	0	32,52,73	0.90	2 (6%)
8	GOL	D	504	-	5,5,5	0.17	0	5,5,5	0.21	0
8	GOL	В	504	-	5,5,5	0.16	0	5,5,5	0.39	0



Mol	Tuno	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FNR	В	502	-	32,33,33	0.47	0	40,50,50	1.09	5 (12%)
5	SF4	В	501	2	0,12,12	-	-	-		
7	NAD	В	503	-	33,39,48	0.65	1 (3%)	38,60,73	0.71	0
3	FES	С	201	1	0,4,4	-	-	-		
3	FES	A	201	1	0,4,4	-	-	-		
8	GOL	В	505	-	5,5,5	0.17	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FNR	D	502	-	-	3/18/18/18	0/3/3/3
7	NAD	D	503	-	-	1/22/42/62	0/3/3/5
5	SF4	D	501	2	-	-	0/6/5/5
8	GOL	D	504	-	-	1/4/4/4	-
8	GOL	В	504	ı	-	1/4/4/4	-
6	FNR	В	502	-	-	9/18/18/18	0/3/3/3
7	NAD	В	503	-	-	3/18/54/62	0/4/4/5
5	SF4	В	501	2	-	-	0/6/5/5
3	FES	С	201	1	-	-	0/1/1/1
3	FES	A	201	1	-	-	0/1/1/1
8	GOL	В	505	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
7	В	503	NAD	C8A-N7A	-2.01	1.31	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
6	В	502	FNR	O5'-C5'-C4'	-3.25	100.67	109.36
6	В	502	FNR	P-O5'-C5'	2.99	126.52	118.30
6	В	502	FNR	O5'-P-O2P	2.63	113.86	106.47
6	В	502	FNR	O3P-P-O5'	-2.63	99.74	106.73
7	D	503	NAD	C5D-C4D-C3D	2.40	117.41	111.80
6	В	502	FNR	O1P-P-O5'	-2.30	100.62	106.73
7	D	503	NAD	C5A-C6A-N6A	2.12	123.58	120.35



There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	502	FNR	N10-C1'-C2'-O2'
6	В	502	FNR	N10-C1'-C2'-C3'
6	В	502	FNR	C3'-C4'-C5'-O5'
6	В	502	FNR	O4'-C4'-C5'-O5'
6	В	502	FNR	C5'-O5'-P-O1P
6	В	502	FNR	C5'-O5'-P-O3P
7	D	503	NAD	C3D-C4D-O4D-C1D
7	В	503	NAD	O4D-C4D-C5D-O5D
7	В	503	NAD	C3D-C4D-C5D-O5D
8	D	504	GOL	O1-C1-C2-C3
6	В	502	FNR	O2'-C2'-C3'-C4'
8	В	505	GOL	O2-C2-C3-O3
6	D	502	FNR	C4'-C5'-O5'-P
6	D	502	FNR	O2'-C2'-C3'-C4'
6	В	502	FNR	O2'-C2'-C3'-O3'
6	В	502	FNR	C5'-O5'-P-O2P
7	В	503	NAD	C5B-O5B-PA-O1A
8	В	504	GOL	O1-C1-C2-O2
6	D	502	FNR	N10-C1'-C2'-O2'

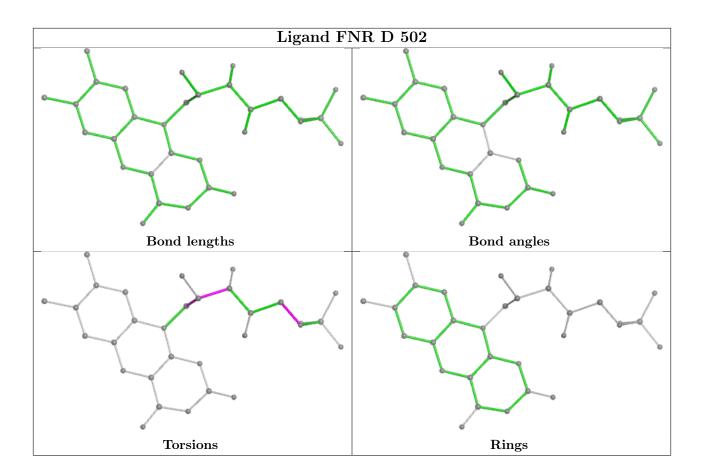
There are no ring outliers.

1 monomer is involved in 2 short contacts:

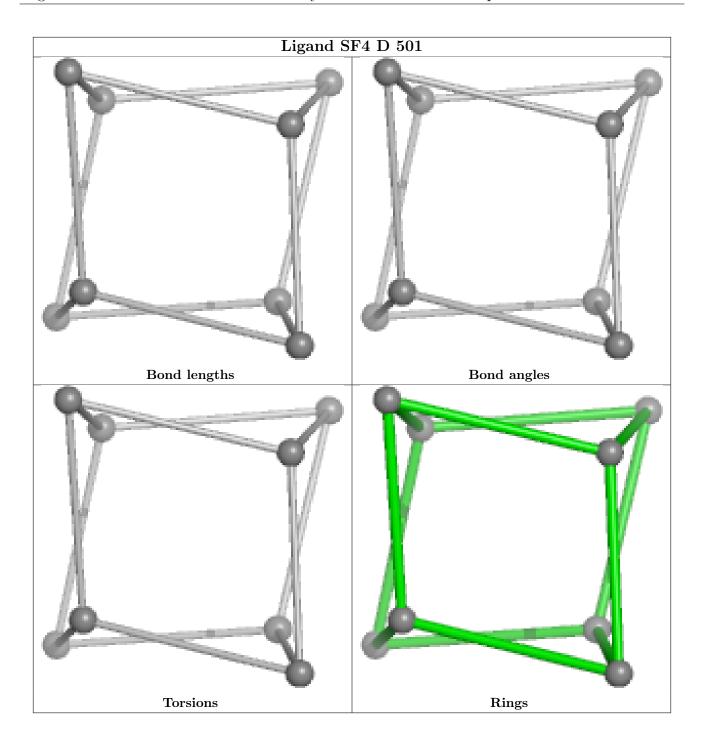
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	В	504	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

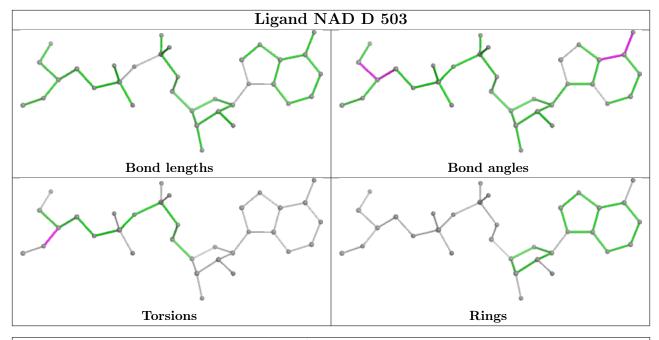


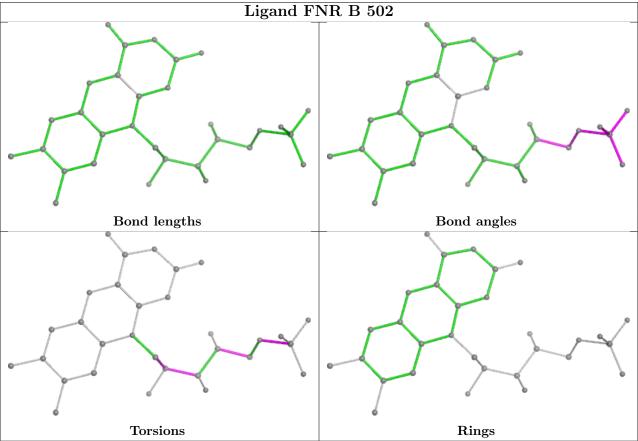




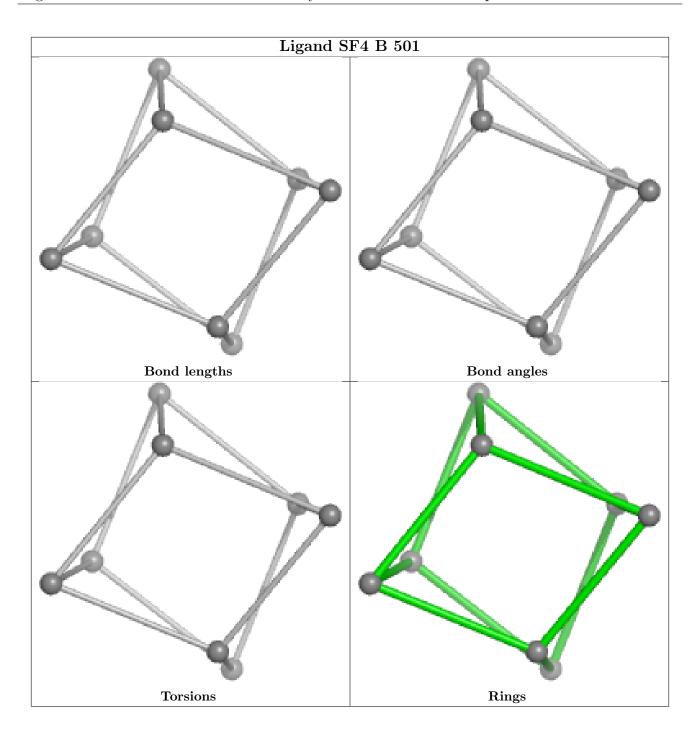




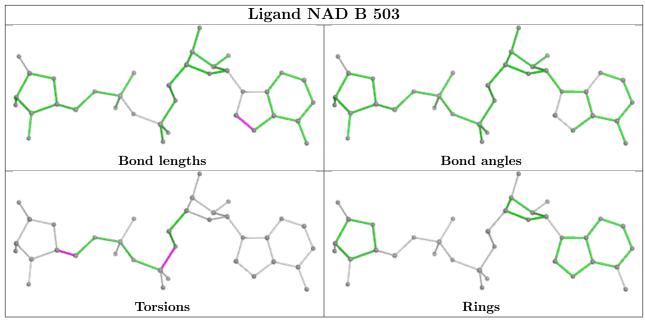


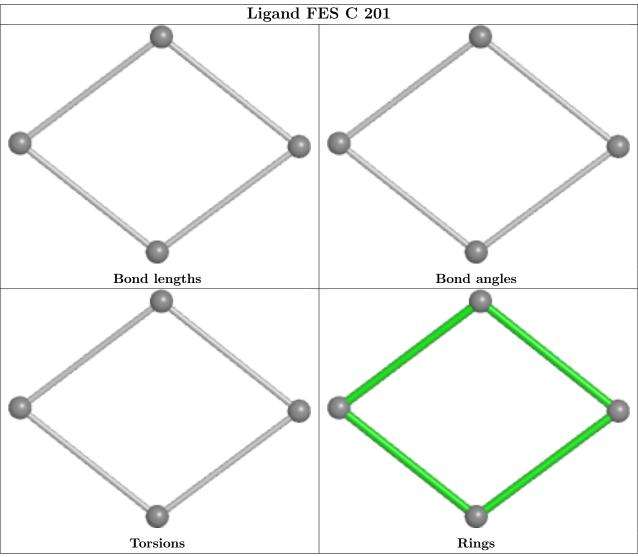




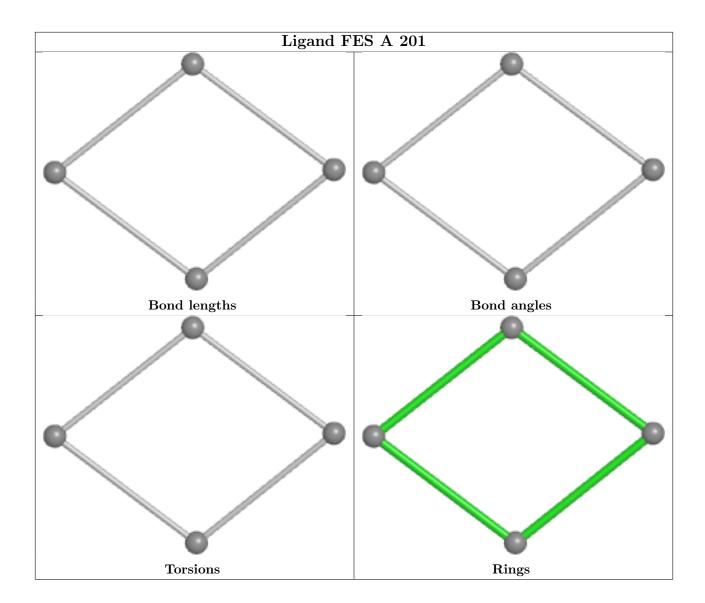












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	156/160 (97%)	0.02	5 (3%) 47 55	11, 24, 44, 78	0
1	С	156/160 (97%)	0.01	6 (3%) 40 47	11, 23, 43, 72	0
2	В	418/434 (96%)	-0.23	7 (1%) 70 76	9, 18, 39, 81	0
2	D	418/434 (96%)	-0.36	2 (0%) 91 94	9, 18, 37, 74	0
All	All	1148/1188 (96%)	-0.21	20 (1%) 70 76	9, 19, 40, 81	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	6.4
2	В	313	PRO	4.7
1	A	6	PHE	4.0
2	D	1	MET	3.3
1	С	54	ASP	2.9
2	В	246	TYR	2.9
2	В	245	ASP	2.8
2	В	242	GLY	2.8
1	С	8	PHE	2.7
1	A	47	GLU	2.3
2	В	314	LEU	2.2
2	В	312	SER	2.1
1	С	5	GLU	2.1
1	С	52	LEU	2.1
1	A	10	GLU	2.1
1	A	14	THR	2.1
1	С	61	ASN	2.1
2	В	315	GLY	2.1
1	С	6	PHE	2.0
2	D	2	ARG	2.0



6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q < 0.9
8	GOL	В	505	6/6	0.69	0.32	49,51,53,56	0
4	NA	В	511	1/1	0.79	0.24	26,26,26,26	0
4	NA	D	507	1/1	0.82	0.15	25,25,25,25	0
4	NA	В	509	1/1	0.85	0.23	37,37,37,37	0
8	GOL	D	504	6/6	0.86	0.15	29,31,35,37	0
4	NA	В	510	1/1	0.88	0.09	35,35,35,35	0
8	GOL	В	504	6/6	0.88	0.19	25,25,25,27	0
9	CL	D	506	1/1	0.88	0.19	64,64,64,64	0
4	NA	D	508	1/1	0.89	0.17	30,30,30,30	0
4	NA	В	508	1/1	0.90	0.15	24,24,24,24	0
4	NA	A	202	1/1	0.91	0.16	22,22,22,22	0
4	NA	В	507	1/1	0.93	0.15	19,19,19,19	0
7	NAD	В	503	36/44	0.94	0.15	19,25,50,55	0
4	NA	С	202	1/1	0.96	0.50	35,35,35,35	0
7	NAD	D	503	33/44	0.96	0.12	16,21,36,42	0
9	CL	D	505	1/1	0.96	0.09	21,21,21,21	0
6	FNR	В	502	31/31	0.96	0.14	10,12,13,14	0
6	FNR	D	502	31/31	0.97	0.13	9,11,12,12	0
9	CL	В	506	1/1	0.98	0.08	14,14,14,14	0
5	SF4	В	501	8/8	0.98	0.05	11,13,13,13	0
4	NA	С	203	1/1	0.98	0.15	12,12,12,12	0
3	FES	A	201	4/4	0.99	0.09	10,11,11,11	0
5	SF4	D	501	8/8	0.99	0.07	11,11,12,12	0
3	FES	С	201	4/4	1.00	0.08	10,10,10,11	0

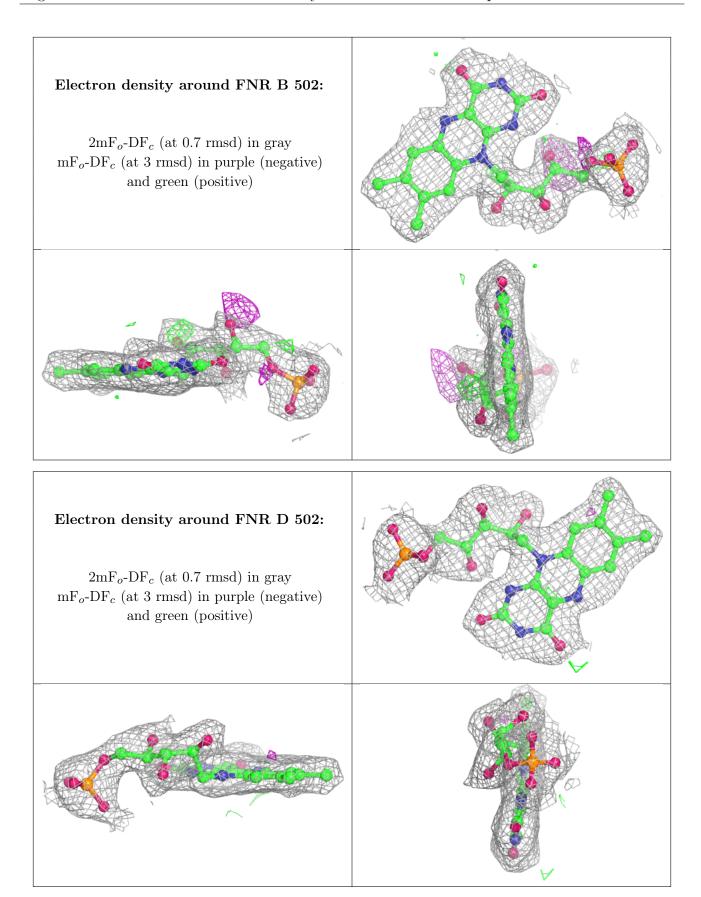
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.

Electron density around NAD B 503: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around NAD D 503: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





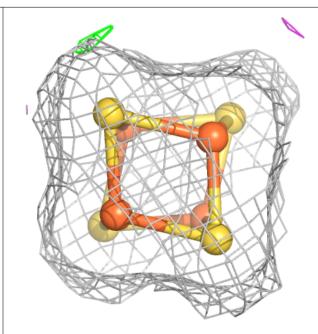


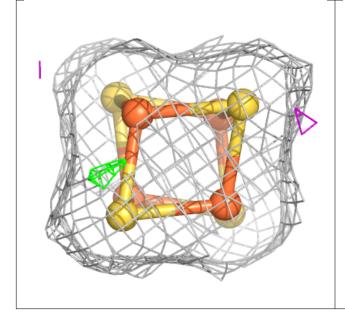


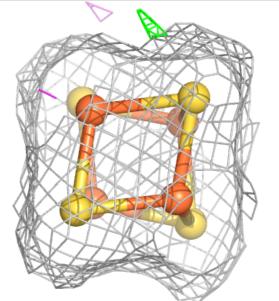


Electron density around SF4 D 501:

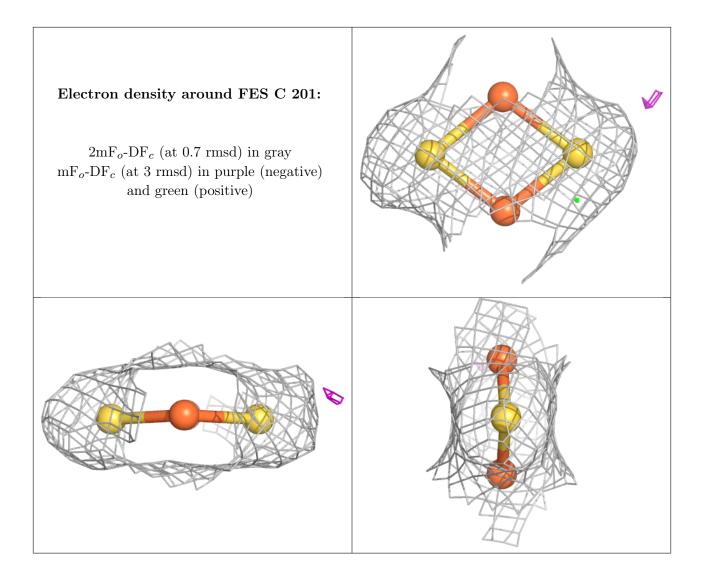
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

